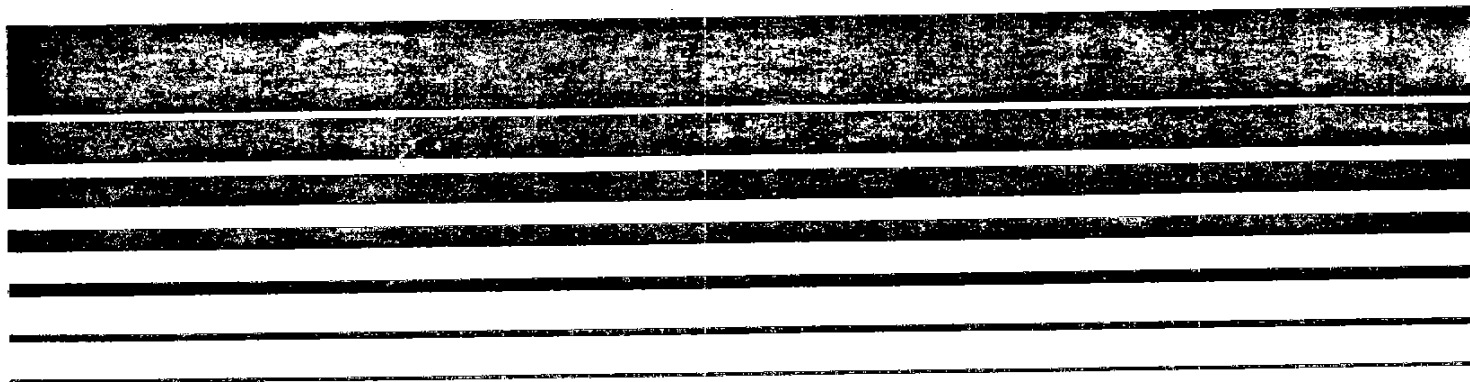




ADDENDUM TO THE USER'S MANUAL FOR OZIPM-4 (PC VERSION)



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USER'S MANUAL FOR OZIPM-4
(PC VERSION)

Office Of Air Quality Planning And Standards
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ABSTRACT

Based on recent studies of the potential effects of biogenic emissions on ozone formation and the effects of biogenics on estimated VOC (volatile organic compounds) control requirements to reach the National Ambient Air Quality Standard (NAAQS) for ozone, the U.S. Environmental Protection Agency (EPA) revised the OZIPM-4 computer code (the computer code associated with the Empirical Kinetics Modeling Approach, EKMA) to treat biogenic emissions independent of the anthropogenic emissions.

Recent studies using three-dimensional photochemical grid models performed by the U.S. Environmental Protection Agency (EPA) on the sensitivity of varying water vapor concentrations on ozone formation showed that ozone levels can vary by as much as 20 to 30 percent with a factor of two variation in water vapor concentrations. Such results have led to concerns of the use of a constant default water vapor concentration of 20000 ppm in the OZIPM-4 computer program associated with the Empirical Kinetics Modeling Approach (EKMA). The U.S. EPA has revised the OZIPM-4 computer code to handle diurnally varying water vapor concentrations.

This report is an addendum to the user's manuals to OZIPM-4 describing the use of new input options to OZIPM-4 to treat biogenic emissions and diurnally varying water concentrations. The use of the "BIOGENICS" option and "WATER" option are available on both the mainframe and personal computer versions of OZIPM-4.

1. INTRODUCTION

Based on recent studies of the potential effects of biogenic emissions on ozone formation and the effects of biogenics on estimated VOC (volatile organic compounds) control requirements to reach the National Ambient Air Quality Standard (NAAQS) for ozone, the U.S. Environmental Protection Agency (EPA) revised the OZIPM-4 computer code (the computer code associated with the Empirical Kinetics Modeling Approach, EKMA) to treat biogenic emissions independently of the anthropogenic emissions.

Biogenic emissions generally vary diurnally as a function of sunlight. Certain biogenic species are emitted from trees even during the nighttime hours. The diurnal patterns are not the same as urban emissions which varies with socio-economic patterns.

This report describes the use of a new input option to OZIPM-4 to treat biogenic emissions. The following subsections describe the use of the "BIOGENICS" option on both mainframe computers and personal computers. The user is referred to Hogo and Gery (1988) and EPA (1987 and 1988) for descriptions of all the options available in OZIPM-4.

Recent studies performed by the U.S. Environmental Protection Agency (EPA) on the sensitivity of varying water vapor concentrations on ozone formation showed that ozone levels can vary by as much as 20 to 30 percent with factors of two variation in water vapor concentrations. Such results have led to concerns of the use of a constant default water vapor concentration of 20000 ppm in the OZIPM-4 computer program associated with the Empirical Kinetics Modeling Approach (EKMA). The U. S. EPA has revised the OZIPM-4 computer code to handle diurnally varying water vapor concentrations.

Chapter 2 and 3 describe the use of a new input option to OZIPM-4 to treat hourly varying water vapor concentrations. These chapters describe the use of the "WATER" option on both mainframe and personal computers. Chapter 2 describes the "WATER" option and the technical basis for calculating water vapor concentrations from ambient temperature and relative humidity measurements. Chapter 3 describes the use of the "WATER" option on personal computers. The user is referred to Hogo and Gery (1988) and EPA (1987 and 1988) for descriptions of all the input options available in OZIPM-4.

BIOGENICS OPTION

The BIOGENICS option is used to input post-0800 emissions of up to five biogenic species. The current photochemical mechanism (CB4) found in OZIPM-4 treats one biogenic species (isoprene) explicitly. Other biogenic species are expressed as CB4 species according to the methodology outlined in EPA (1987) and Hogo and Gery (1988). The inputs to the BIOGENICS option are listed in Table 1-1. The first line in the BIOGENICS option contains the four letter code "BIOG" to invoke the BIOGENICS option followed by the number of hours of emissions of the biogenic species. Note, a negative value is entered to be consistent with the EMISSIONS and MASS options. The third item on the first line is the number of biogenic species with post-0800 emissions. Up to five biogenic species can be input. The initial mixing height (in meters) is entered next. The mixing height is used to convert hourly emission densities to concentration units required by the OZIPM-4 program.

The next set of lines (lines 2 to 5) are repeated for each biogenic species up to the number specified in columns 21-30 of the first line. The second line of the BIOGENICS option contains the name of the biogenic species. The only biogenic species which requires an exact spelling is isoprene (ISOP) since it is a species found in the photochemical mechanism. Note that ISOP must be in capital letters. The next item (located in columns 11-20) on the second line contains a flag to tell OZIPM-4 that the species is treated explicitly in the photochemical mechanism. A nonzero positive value would tell OZIPM-4 that the species is to be treated as a mixture of CB4 species. Currently, for isoprene, the flag would be set to zero. If the user wishes to treat isoprene as a mixture of CB4 species, then a nonzero flag can be entered in this field. The next items on line 2 are the present-day biogenic concentrations transported in the surface layer and entrained from aloft (in units of ppm). The percent change in biogenic emissions for the future year is entered next, followed by the future-year concentrations transported in the surface layer and entrained from aloft.

The third line of the BIOGENICS option contains the species molecular weight in units of gm/mole. If the flag located in columns 11-20 of line 2 is nonzero, the next lines contain the species bond fractions apportioned to the CB4 species. The bond fractions must be inputted in the following order: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, and NR. A list of commonly occurring biogenic species along with their molecular weights and bond fractions are listed in Table 1-2 as a quick reference.

TABLE 1-1. BIOGENIC option (Continued)

Option	Line No.	Column	Contents
		21-30	Present-day concentration transported in the surface layer (DF=0)
		31-40	Present-day concentration transported aloft (DF = 0.0)
		41-50*	Percent change in biogenic emissions for the future year
		51-60*	Future-year concentration transported in the surface layer (DF=0)
		61-70*	Future-year concentration transported aloft (DF = 0.0)
		71-80	Not read
	3+	1-10	Species molecular weight (Units of gm/moles)
	4+ (optional)	1-10 11-20	If a nonzero value is entered on columns of line 2, the species profiles by bond group of the biogenic species is entered here.
		11-20	The species profiles should be in the following order: ETH, OLE, ALD2, FORM, TOL, XYL, PAR, and NR.
		.	.
		.	.

*Not used with CALC and ISOP options.

TABLE 1-1. BIOGENIC option (Continued)

Option	Line No.	Column	Contents
		61-70	Continue on next line (if necessary).
		71-80	Not read
5+	1-10		Present-day hourly biogenic emissions (kg/km ²)
	11-20		(continue on next line if necessary)
	.		.
	.		.
	.		.
		61-70	

The next set of lines in the BIOGENICS option contains the hourly emission densities in units of kg/km^2 . Note, the BIOGENICS option can be used to input only initial and aloft biogenic concentrations by entering small emission densities (e.g., 0.00001) for each of the hours of emissions.

USING THE BIOGENICS OPTION ON THE PC SYSTEM

The personal computer (PC) version of the OZIPM-4 program contains a front-end interface which allows the user to enter the input parameters through a series of pop-up menus (EPA, 1988). The front-end interface was modified to handle the BIOGENICS option. This section describes how to access the BIOGENICS option on the PC system. To access the OZIPM-4 on the PC system, type OZACCESS. A menu will appear on the monitor. Choose the Edit option as described in the user's manual (EPA, 1988). A new screen will appear as shown in Figure 1-1. To access the BIOGenics option, hit the Q key or by using the up or down arrow keys to position to the BIOGenics option and hit the ENTER key. The BIOGenics option screen will be displayed (see Figure 1-2). The BIOGenics option contains three main inputs (the number of hours of biogenic emissions, the number of biogenic species, and the initial mixing height). Upon entering the number of hours of biogenic emissions, the data fields for the emission values will be displayed (Figure 1-3). The middle portion of the menu shows the input parameters for each of the biogenic species. Choose the species to edit or view by entering a number representing the order of the biogenic species (e.g., if terpenes is the first species, then enter 1, etc). Enter the input values for the current biogenic species by using the TAB or arrow keys to move around the menu. Blanks in any of the fields will be interpreted as zeroes. Be sure to hit the ENTER key after typing a value so that the OZIPM-4 system will accept the value. After entering all values, hit the F10 key so that the OZIPM-4 system can accept the option.

Table 1-2

MOLECULAR WEIGHTS AND SPECIES BOND FRACTIONS
OF SOME COMMON BIOGENIC SPECIES

Species	Molecular Weight	ETH	OLE	ALD2	FORM	TOL	XYL	PAR	NR
A-Pinene	136.24	--	0.5	1.5	--	--	--	6.0	--
B-Pinene	136.24	--	1.0	--	--	--	--	8.0	--
3-Carene	136.23	--	2.0	--	--	--	--	6.0	--
d-Limonene	136.24	--	1.0	2.0	--	--	--	4.0	--
Isoprene	68.13	--	2.0	--	--	--	--	1.0	--
Terpenes	136.24	--	1.0	--	--	--	--	8.0	--

Edit	Load/save	Run	Plot	Directory	Quit
------	-----------	-----	------	-----------	------

A PLACe B DILution C TEMPerature D TRANSport E MASSemis F REACTivity G CREDit H TITLe I TIME J SPECies K ACCUracY L ALREAdy M PLOT N EKMA O CALCulate P ISOPleth Q BIOGenics R WATER

Prompt PLACE: set the location for this simulation

↑ ↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 1-1. Example screen display of the 17 input options (including the BIOGenics option) available in OZIPM-4.

BIOGENICS Allow for post-0800 biogenic emissions. If the BIOG
---- option is not used, defaults are no post-0800 biogenic emissions,
and no transported surface and aloft concentrations of biogenics.

Hours: Species: Height:

Number of species to view/edit:	1 Name:	Molwt:
CB4 flag:	Present surface:	Aloft:
Future change:	Future surface:	Aloft:

Species Profile (fill in only if CB4 flag equals 1)

ETH:	OLE:	ALD2:	FORM:
TOL:	XYL:	PAR:	NR:

Hourly emissions--

Enter the number of emission hours

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 1-2. Example screen display of the BIOGenics option menu.

BIOGENICS Allow for post-0800 biogenic emissions. If the BIOG
---- option is not used, defaults are no post-0800 biogenic emissions,
and no transported surface and aloft concentrations of biogenics.

Hours: 11 Species: Height:

Number of species to view/edit: 1 Name: Molwt:
CB4 flag: Present surface: Aloft:
Future change: Future surface: Aloft:

Species Profile (fill in only if CB4 flag equals 1)

ETH: OLE: ALD2: FORM:
TOL: XYL: PAR: NR:

Hourly emissions--

1: 2: 3: 4: 5: 6:
7: 8: 9: 10: 11:

Enter the number of biogenic species (DF=0)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 1-3. Example screen display of the BIOGenics option menu
with hourly emission fields.

2. IMPLEMENTATION OF VARYING WATER CONCENTRATIONS TO OZIPM4

Ambient water concentrations can be estimated using the Clausius-Clapeyron equation which describes the solidification, melting, and evaporation of water as a function of temperature. The Clausius-Clapeyron equation is a well-known equation of water vapor pressure (Hess, 1959) and is expressed as follows:

$$de_s/dT = L_{12}/T(a_2 - a_1)$$

where e_s is the equilibrium vapor pressure, T is the temperature, L_{12} is the latent heat of the phase change, and a is the volume. From Hess (1959), equation (1) can be solved for the water concentration and described as follows:

$$H_2O = 6030(0.01)(rh)/pres]e^{[R*(1/273-1/T)]}$$

where rh is the relative humidity (percent), $pres$ is the ambient pressure (atms), and R is

6133.17 when T is below 273 K and

18.02[597.3 - .566(T - 273)]/1.9869
when $T \geq 273$ K.

WATER OPTION

The WATER option is used to input hourly varying relative humidities in percent. The relative humidities are used along with the ambient temperature to calculate the water vapor concentrations as discussed above. The inputs to the WATER option are listed in Table 2-1. The first line in the WATER option contains the four letter code "WATE" to invoke the WATER option. The next parameter on line 1 is the number of hours with varying water concentrations. The third parameter on line 1 is the atmospheric pressure in inches of mercury (Hg). The relative humidity values at the beginning of each hour are then entered (beginning on line 2) for each hour and at the end of the last hour with varying water concentrations. Therefore, if there are n hours with varying water concentrations, $n+1$ relative humidities are entered. Up to 24 hours of relative humidity values may be entered. Note that the WATER option must follow the TEMPERATURE option in the input list in order for the OZIPM-4 program to recognize varying temperature profiles.

TABLE 2-1. WATER option

Option	Line No.	Column	Contents
WATER			Allows for varying water concentration profile. This option must follow the <u>TEMP</u> erature option. Information is entered regarding the number of hours with varying water concentrations, the hourly relative humidity, and the atmospheric pressure. The relative humidity values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 relative humidity values. If the WATE option is not used, the default water concentration is 20000 ppm.
	1	1-4	WATE (DF = 20000 ppm)
		11-20	Number of hours of varying water concentrations. (MAX = 24)
		21-30	Enter the atmospheric pressure; units of inches of Hg. (DF=29.92 inches of Hg which is equal to 1 atm)
	2	1-10	Relative humidity (in percent) at time t = 0
		11-20	Relative humidity at time t = 1 hr
		21-30	Relative humidity at time t = 2 hr
		31-40	Relative humidity at time t = 3 hr
		41-50	Relative humidity at time t = 4 hr
		51-60	Relative humidity at time t = 5 hr
		61-70	Relative humidity at time t = 6 hr
		71-80	Not read
	3+ (optional)	1-10	Continuation of relative humidity values
		.	.
		.	.
		.	.
		61-70	
		71-80	Not read

3. USING THE WATER OPTION ON PC SYSTEMS

The personal computer (PC) version of the OZIPM-4 program contains a front-end interface which allows the user to enter the input parameters through a series of pop-up menus (EPA, 1988). The front-end interface was modified to handle the WATER option. This section describes how to access the WATER option on the PC system.

To access the OZIPM-4 on the PC system, type OZACCESS. A menu with five options across the top of the screen will appear on the monitor. Choose the Edit option as described in the user's manual (EPA, 1988). A new screen will appear as shown in Figure 3-1. To access the WATER option, hit the R key or by using the up or down arrow keys to position to the WATER option and hit the ENTER key. The WATER option screen will be displayed as shown in Figure 3-2. The WATER option contains two main inputs (the number of hours with varying water concentrations and the atmospheric pressure). Upon entering the number of hours with varying water concentrations, the data fields for the relative humidity values will be displayed (Figure 3-3). Use the TAB or arrow keys to move around the menu and enter the input values. Remember to hit the ENTER key after each entry in order to retain the value. Blanks in any fields will be interpreted as zeroes. Be sure to hit the F10 key after entering all values so that the OZIPM-4 system can accept the option.

Edit	Load/save	Run	Plot	Directory	Quit
A PLACe B DILUtion C TEMPerature D TRANSport E MASSEmis F REACTivity G CREDit H TITLe I TIME J SPECies K ACCURacy L ALREady M PLOT N EKMA O CALCulate P ISOPleth Q BIOGenics R WATER					
<div style="text-align: right;">Prompt</div> PLACE: set the location for this simulation					
↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear					

Figure 3-1. Example screen display of the 18 input options (including the WATER option) available in OZIPM-4.

WATER Allows for varying water concentrations during the simulation. If
---- this option is not used, the concentrations default to 20,000 ppm

Hours:

Pressure:

Enter the number of hours of varying relative humidity (1-24)

↑↓ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 3-2. Example screen display of the WATER option menu.

WATER Allows for varying water concentrations during the simulation. If
---- this option is not used, the concentrations default to 20,000 ppm

Hours: 10

Pressure:

0:	1:	2:	3:	4:	5:
6:	7:	8:	9:	10:	

Enter the percent relative humidity for this hour

↑ :Locate Enter:Enter F1:help F10:Accept ESC:Reject F9:Clear

Figure 3-3. Example screen display of the WATER option menu with hourly relative humidity fields.

REFERENCES

EPA (1987), "Guidelines for use of City-Specific EKMA in Preparing Post-1987 Ozone SIP's", U.S. Environmental Protection Agency, Research Triangle Park, North Carolina.

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Hess, S.L., (1959), "Introduction to Theoretical Meteorology", Holt, Rinehart and Winston, New York, New York.

Hogo H., and M. W. Gery (1988), "User's Guide for Executing OZIPM-4 with CBM-IV or Optional Mechanisms", Volume I, SYSAPP-88/001, Systems Applications, Inc., San Rafael, California.

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16. ABSTRACT OZIPM-4 is a model which allows the user to estimate the volatile organic compound (VOC) control requirement for a city in order to achieve the national ambient air quality standard for ozone. This manual describes two new options that have been added to OZIPM-4. The first option (BIOG) allows the user to input biogenic emission rates. The other option (WATE) allows the user to estimate hourly atmospheric moisture content.		
17. KEY WORDS AND DOCUMENT ANALYSIS		
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